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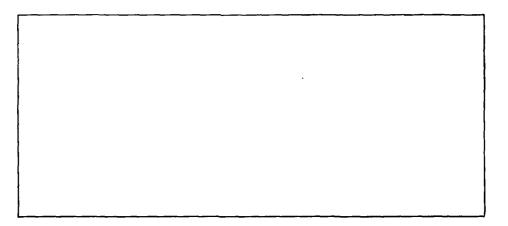


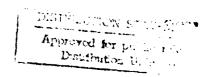
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YALE UNIVERSITY
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PRECONDITIONED CONJUGATE-GRADIENT METHODS FOR NONSYMMETRIC SYSTEMS OF LINEAR EQUATIONS

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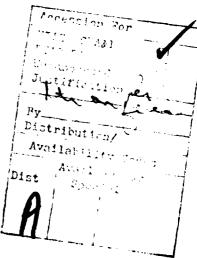
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Introduction

In this paper, we present a class of iterative decent methods for colving large, sparse, nonsymmetric systems of linear equations whose coefficient matrices have positive-definite symmetric parts. Such problems commonly arise from the discretization of non-welf-adjoint elliptic partial differential equations. The methods we consider are modelled after the conjugate gradient method (CG) 41.46. They require no estimation of parameters and their rate of convergence appears to depend on the appearum of A rather than 47. Their convergence can also be accelerated by precombitioning techniques.

The methods are tested on two sample problems, and their numerical behavior is compared with that of two other mith'ds, the menyametric Chebyshev algorithm [10, 11], and the comjugate gradient method applied to the mernal equations [8, 9, 13]. All the methods are tested in conjunction with two preconditionings, the incomplete LW factorization [12], and the modified incomplete LW factorization [12], and the modified incomplete LW factorization [12], and the modified

In Section 2, we describe the methods, outline their computational costs, and present some bounds on their convergence rated. In Section 3, we show how they can be implemented with preconditioning techniques. In Section 4, we describe two sample nonsymmetric model problems derived from a now sail adjoint elliptic equation. Finally, in Section 5, we present the results of numerical experiments with the methods. Tables and figures follow the list of references.



2. The Generalized Conjugate desidual Method, and Varianta

In this section, we describe a class of descent methods for solving the linear system

where A is a nonsymmetric matrix of order N with positive definite symmetric part. We consider four variants, all of which have the following form:

Choose 
$$z_0$$
 . Compute  $z_0$  .  $f = Az_0$  . Set  $p_0$  =  $z_0$  . For  $z_0$  .

The shoice of  $a_1$  minimizes  $B_2 - h(x_1 \cdot ap_1) B_2 = B_{1+1} B_2$  as a function of a, so that the Bucklean norm of the residual decreases at each step. The four methods are determined by four techniques for choosing  $p_{1+1}$ :

(1) Generalized Conjugate Residuel (OCR):

$$p_{j+1} = r_{j+1} + \sum_{j=0}^{j} b_j^{(1)} p_j$$
 (2.2)

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$$b_{j}^{(1)} = -\frac{(Ax_{j+1} \cdot Ay_{j})}{(Ay_{j} \cdot Ay_{j})}$$
,  $j \le 1$  . (2.3)

(2) Orthonin(k) [118]:

$$P_{i+1} = F_{i+1} = \frac{1}{j-\max\{0, i, k+1\}} \frac{b_{i}}{j} \quad ,$$
 where  $\{b_i^{\{1\}}\}$  are defined by  $\{2,3\}$ .

. (CECE) :

The generalized conjugate residual algorithm restarted every bil steps. Every bil steps, the current iterate,  $a_{j(k+1)}$  in takem as the new starting guess,

(4) Minimum Residual (MR): Pi+1 " Fi+1 .

The direction vectors (p) generated by GCE are constructed so that

As a result, x, minimizes the functional E(v) - Mr-Auly over the affine space  $x_0$  + span(p\_0.....p\_{s-1}), and

OCE is the maslogue of the conjugate residual method (CE) [2, 15] for symmetric problems. If A is symmetric and positive-definite, then (2.2) reduces to a two-term expression and the resulting algorithm is equivalent to

Orthomia(k) has been proposed as an alternative to GCE that is less expensive in terms of both work per iteration and storage. The vector  $\mathbf{p}_{1:1}$  is orthogonal to only the last k (2 0) vectors  $\{\mathbf{p}_j\}_{j=1,k+1}^{J}$ . Only k direction vectors need to be stored. The iterate  $\mathbf{x}_j$  minimizes  $\mathbf{E}(\mathbf{v})$  over the affine been  $\mathbf{x}_k$  - spenip.  $k-1,\dots,p_{j-1}$ .

GCR(k) is also proposed as a less expensive site insite to GCR. As in Orthomin(k), at most k direction vectors have to be assed. The cost periteration is lower, since in general fewer than k direction vectors are used to compute  $\mathbf{p}_{k+1}$ .

MR corresponds to the special case of k=0 for both Unithmin(k) and GCR(k). It has very modest work and storage requirements, and in the symmetric case resembles the method of steepest descent.

In Table 2-1, we summarize the work and storage costs (excluding storage for A) of computing  $\mathbf{x}_i$  for each of the methods. The storage for GCR includes apace for the vectors,  $\mathbf{x}_i$ ,  $\mathbf{x}_i$ ,  $\mathbf{A}_{i}$ ,  $\mathbf{P}_0$ ,..., $\mathbf{P}_{i}$ , and  $\mathbf{A}_{i0}$ .... $\mathbf{A}_{P_{i-1}}$  Ap<sub>i</sub> is computed recursively as

$$Ap_1 = Ar_1 + \frac{1-1}{2} b_1^{(1-1)} Ap_j$$
.

to that the only matrix-vector product required is Ar<sub>1</sub>. The satries for Orthonin(k) correspond to the requirements after the b'th iteration. The work for GCE(k) is the average over k+1 iterations.

GCR gives the exact solution to (2.1) in at most N iterations. The three variants do not in general display finite termination. In practice, however, all four methods tend to compute sufficiently accurate solutions in far fewer than N iterations.

We now present some error bounds for the four methods. Let  $R:=(A^*A^T)/2$  denote the symmetric part of  $A_*$  and let  $R:=-(A^*A^T)/2$  denote the above-symmetric part of  $A_*$  so that A=M:R. Let  $J:=T^{-1}A$  I denote the Jordan canonical form of  $A_*$  for any square matrix  $J_*$  let  $\sigma(J_*)$  denote the set of eigenvalues of  $J_*$  let  $\lambda_{M,N}$  denote the eigenvalue of  $J_*$  is an allest absolute

value, let  $\lambda_{max}(1)$  denote the eigenvalue of largest absolute value, and let p(1) denote the specifial radius of X.  $\lambda_{max}(1)$ . If X is nonstagular, let K(1) denote the condition number of X, defined to be  $K(2):=R\lambda_{2}^{2}R^{-1}$  franch; let  $P_{1}$  denote the set of real polynomials  $q_{1}$  of degree less than or equal to 1 such that  $q_{1}(0)=1$ .

The following bounds for Gilt and Gilt(h) are proved using (2.4):

Decres 2.1: If | f | is the sequence of residuals generated by UCE, then

If A has a complete set of eigenvectors, then

. .

Moreover, if A is normal. then

Theorem 2.2: If  $\{r_j\}$  is the sequence of residuals generated by  $\operatorname{GCR}(k)$ , then

$$\| \mathbf{r}_{j \, (k+1)} \|_{2} \leq \{ \max_{q_{k+1}} \| \mathbf{u}_{q_{k+1}}(\mathbf{a}) \|_{2} \}^{j} \| \mathbf{r}_{0} \|_{2}$$

If A has a complete set of eigenvectors, then

$$\| f_{1}(k+1) \|_{2}^{2} \le (K(T)) \| f_{k+1} \|^{1} \| f_{0} \|_{2} \quad ,$$

and if A is normal, then

$$B_{r_j(k+1)} \|_2 \le (a_{k+1})^{\frac{1}{2}} B_{r_0} B_2.$$

Finally, the fullowing result implies that Orthomistal converges, and provides another error bound for GCR, GCR(b), and MK.

Theorem 2.3: If  $\{r_{i}\}$  is the sequence of residuals generated by GCR, Orthomia(k), GCR(k), or MR, then

$$\| \mathbf{r}_{i} \|_{2} \le \left[ 1 - \frac{\lambda_{\min}(\mathbf{H})^{2}}{\lambda_{\max}(\mathbf{A}^{T}\mathbf{A})} \right]^{1/2} \| \mathbf{r}_{0} \|_{2}$$

å

$$\mathbb{E}_{1}\mathbb{I}_{2} \leq \left[1 - \frac{\lambda_{\min}}{\lambda_{\min}(\mathbb{H})\lambda_{\max}(\mathbb{H})} - \frac{1}{\rho(\mathbb{R})^{2}}\right]^{1/2} \mathbb{E}_{0}\mathbb{I}_{2}$$

Proofs of these results can be found in [4].

## 3. Implementation with Preconditioning

The methods presented in the previous section can be accelerated by preconditioning techniques. Let Q be some nonsingular matrin. The solution to (2.1) can be found by solving any of the alternative problems

$$\tilde{A}_{\tilde{X}_{n}} = \{q^{-1}A\} \{z\} = \{q^{-1}f\} = \tilde{Y}$$
; (3.1)

$$\tilde{K} = [A \ q^{-1}] \ \{q_x\} = \{f\} \approx \tilde{f}$$
; (3.2)

$$\tilde{A} \tilde{x} = [q_1^{-1} A \ q_2^{-1}] [q_2 x] = [q_1^{-1} f] = \tilde{f}$$
 ; (3.3)

where Q is (formally) factored into the product  $Q_1Q_2$  . It systems of equations having Q as coefficient matrix can be solved easily, then the use of Q as

preconditioning may greatly speed the convergence of GCK and its varients. In this section, we discuss the implementation of preconditioned versions of the four methods.

Ma-1(f-An1) M2 is minimized at each step. The residual of (3.2) is the same as applying the preconditioning. For example, if GCR is applied to (3.1), then preconditioning is used, the quantity minimized depends on the technique of the residual of the original problem (2.1). In this paper, we restrict our minimize the Euclidean norm of the residual over some subspece. Then At each atep, the approximate solutions generated by GCE et. al. attention to this version of the preconditioned problem.

GCR can be implemented to solve (2.1) using (3.2) as follows:

Algorithm 2.1.: The preconditioned generalized conjugate residual method:

Choose x<sub>0</sub> .

Compate ro = f - Ano

Set Po = 'Co .

FOR 1 - 0 STRP 1 UNTIL Convergence DO

$$s_1 \sim \frac{(r_1, Ap_1)}{(Ap_1, Ap_1)}$$

Riel = Zi + BiPi

$$b_{j}^{\{1\}} = \frac{(Au^{-1}r_{i+1}, Ap_{j})}{(Ap_{j}, Ap_{j})}, \quad j \leq i$$

$$P_{i+1} = Q^{-1}r_{i+1} + \frac{1}{j=0} b_j^{(1)}p_i .$$

replaced by a preconditioned matrix-vector product Alt I [1]. In general, this operation is performed in two steps: a system of equatious with coefficient metrix Q is solved for  $Q^{-1} \Gamma_{1+1}$ , and the result is multiplied by A. For some preconditionings based on the incomplete factorization of A, more efficient The work per iteration for preconditioned GCR in identical to that for the unpreconditioned vertion, except that the matrix vactor product is techniques for porforming this operation have been developed isl.

requires one more vector of storege than the unprecenditioned version, for In addition to the extra storage required for Q, preconditioned

Algorithm 3.1. For all three methods, the work per iteration differs from the The implementations of Orthonin(k), GCR(k), and MR are analogous to unpreconditioned versions only in the cost of the matrix vector product. Again, extra storage is required for Q and Q -1

## 4. Sample Problems

In this section, we describe two sample problems on which we tested the methods. Consider the elliptic differential equation

$$- (u_{xx} + u_{yy}) + \beta u_{x} = 0 , (4.1)$$

on the quarter plane x > 0, y > 0, with boundary conditions

$$u(x,0) = 0$$
 ,  $u(0,y) = 1$  , (4.2)

For large \$, the solution u has a boundary layer near y - 0, and is nearly equal to 1 elsewhere [7].

For the numerical solution of (4.1) and (4.2), we restrict the domain to the unit square (0,1) x (0,1), and impose the additional boundary conditions

$$u(s,t) + t$$
 ,  $u_{k}(1,y) + 0$  . (4.3)

The effect of the outflow boundary condition is to make the boundary layer in the namerical solution nemoccillatory [7]. The exect solution to

(4.1) - (4.3) is not known. A two-dimensional representation of a numerical solution for  $\beta$  = 100 is shown in Figure 4-1.

For the first test problem, we discretize

For the first test problem, we discretize (4.1) using contered finite differences on a uniform a x n grid, with h  $\frac{1}{n+1}$  [17]. The right boundary condition is discretized by

Let  $\mathbf{u}_{i,j}$  denote the approximation to  $\mathbf{u}(i\mathbf{h},j\mathbf{h})$ . The difference equations for the discretized problem are then

$$4u_{i,j} - u_{i,j-1} - (1 + \frac{\beta h}{2})u_{i-1,j} - (1 - \frac{\beta h}{2})u_{i+1,j}$$

$$(3+\frac{\beta h}{2})_{n_{1}} - a_{n,\,j-1} - (1+\frac{\beta h}{2})_{n-1,\,j} - a_{n,\,j+1} = 0 \ ,$$

where

$$u_{ij} = \begin{cases} 0 & j = 0 \end{cases}$$
 (4.5)

If the unknowns uj are ordered in the natural row-by-row menner, then

(4.4) can be expressed as an N x N block tridiagonal system of linear equations

$$A \times 1^{-1} - \frac{T_1 - W_1}{V_2 - T_2} = \frac{1}{W - f}, \qquad (4.6)$$

where for 1 & 1 & n. T, is the n z n tridisgonal metria

and  $V_{\underline{1}}$  and  $W_{\underline{1}}$  are a. n. identity matrices. The right hand side f is determined by (4.5), and  $N=n^2$ . A is a nonsymmetric matrix, and it has complex eigenvalues for  $\overline{P_0}>1$  [14].

For the second test problem, we resolve the boundary layer by introducing the change of coordinates

$$y(\eta) = y'_0 \eta + (1 - y'_0) \eta^4$$

[16], with  $y_0' = \frac{1}{\beta}$ . Letting  $v(x,\eta) := u(x,y(\eta))$ , equation (4.1) becomes

$$- \left\{ v_{xx} + \frac{1}{y^*} (\frac{1}{y^*} v_{y})_{\eta} \right\} + \beta v_{x} = 0$$

with boundary conditions

$$v(x,0) = 0$$
 ,  $v(0,\eta) = 1$ 

$$v(x,1) = 1$$
 ,  $v_{x}(1,\eta) = 0$  .

Using a uniform a s n grid on the unit (x,n) aquare, with b ,  $\frac{1}{n^2 3}$  , and  $y_j^*=y^*(jb)$  , the difference equations are

=

$$\frac{(2+\frac{1}{y_1^2})^{\frac{1}{y_1^2+1/2}}}{(1+\frac{p_1^2}{y_1^2+1/2})^{\frac{1}{y_1^2+1/2}}} \frac{1}{y_1^2+1/2} \frac{1}{y_1^2+$$

$$(1+\frac{1}{y_j^2}(\frac{1}{y_j^{1+1/2}}+\frac{1}{y_j^{1+1/2}}+\frac{1}{y_j^{1+1/2}})+\frac{jh}{2})^{n_j}-\frac{1}{y_j^{1}}\frac{1}{y_j^{1+1/2}}^{-1}^{n_j}-\frac{1}{1}-(1+\frac{jh}{2})^{n_j}_{n_j}+1,j} \\ -\frac{1}{y_j^{1}}\frac{1}{y_j^{1+1/2}}^{-1}^{-1}^{-1}^{-1}-0 \ , \qquad 1 \le j \le n \ .$$

The resulting matrix equation is also of block tridingonal form (4.6), and aonsymmetry occurs in both sets of diagonals. Because  $y_j^i$  is small for justs 0, the diagonal coefficients in  $T_j$ ,  $V_j$ , and  $V_j$  are large for small j.

## 5. Mmerical Experiments

In this section, we present the results of numerical experiments. We solved the discrete problems (4.4) and (4.7) with  $h=\frac{1}{32},\frac{1}{48},$  and  $\frac{1}{64}.$  The linear systems are of order N = 961, 2209, and 3969. Three values of  $\beta$  were used,  $\beta$  = 10, 100, and 1000. All computations were done in double precision on a DECSYSTEM=20.

We tested the algorithms MR. Orthomin(1), Orthomin(5), GCK(1), and GCE(5). We also used the nonsymmetric Chebyshev algorithm [10, 11], and the conjugate gradient method applied to the normal equations (CGN) to a olve the

same set of problems. The cost per iteration of the Chebyshev signrithm is 2N multiplications plus one matrix-vector product. The uverhead required by the Chebyshev signrithm for estimating eigenvalues is not included in the operation counts. The cost per iteration of CGN is 5N multiplications plus two matrix-vector products.

All of the methods were tested in conjunction with two preconditionings: the incomplete LU factorization (ILU) [12], and the modified incomplete LU factorization (MILU) [3, 6]. The preconditioned problems were formulated as in (3.2); this means that the variational quantity minimized by all the GCE-variants, as well by GGN, is the Euclidean norm of the residual of the original linear problem, Er<sub>1</sub>E<sub>2</sub>.

The ILV factorization is an approximate LV factorization of A into  $\mathbf{q}_1 = \mathbf{L}_1 \mathbf{v}_1$  that satisfies

2. if 
$$A_{ij} \neq 0$$
, then  $[Q_I]_{ij} = A_{ij}$ .

That is, the approximate factors are as sparse as the luwer- and upper-triangular parts of A, respectively, and the product  $\mathbf{q}_1$  agrees with A in the nonzero entries of A.

The MLLU factorization is an approximate LU factorization into  $\mathbf{Q}_M = \mathbf{I}_M \mathbf{U}_M$  that satisfies

1. if 
$$A_{ij} = 0$$
, then  $\{i_M\}_{i,j} = 0$  and  $\{u_M\}_{i,j} = 0$ ;

2. If Aij # O, and i # j, then 
$$\{Q_{ij}\}^{\perp} A_{ij}$$
.

MILU differs from 1LU in that the diagonal of  $Q_M$  is modified so that for  $1 \le 1 \le N$  .

$$\sum_{j=0}^{N} (A_{ij} - \{Q_{ij}\}_{ij}) = 0 ...$$

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The preconditioned matrix vector products were implemented to take advantage of the two cyclic nature of the problems [3]. The cost of a preconditioned matrix-vector product is 9N multiplications. The atopping criterion for all the tests was

Tables 5-4, 5-5, and 5-6 show the number of multiplications needed by each of the methods to satisfy the stopping criterion for Problem 2 (4.7). Figures 5-7 through 5-12 graph residual norm against multiplications for Problem 2, with h =  $\frac{1}{4g}$ .

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Table 2-1 Work per iteration (see denotes a matrix vector product) and atorage requirements of GCM and variants.

	_ ਤੁ	Orthomin(k)	(4) NO 1	#
Work/ (31+4)N	N(++15)	Work/   (31+4)N   (3k+4)N   ((3/2	((3/2)1·4)N	*
	À	-	` .	· · · -
Storage   (21+3)N	(21+3)N	Storage   (21+3)N   (2h+3)N   (2h	(2k+3)N	38

Pigure 4-1 Mamoritani nolution tu (4.1) (4.3) for p = 100

Table 5-1: Work required to reduce relative residual by factor 1.k b.  $Problem\ 1,\ \text{fole}\ \sim\ 10$ 

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		3				
43	32	<b>*</b>	3	32	₽	3
	1432409	7006113	>15000000	373921	1290477	3041573
Orithmeta (1)	958493	3931397	10991957	275253	810701	1712141
Orthusto (5)	1057269	3236541	8369493	389069	1204533	2609973
(0,000)	784989	3658793	11454393	279681	864793	1860061
608(5)	734829	2774717	6451161	329277	974477	2077701
CGN	1775376	8325204	>18000000	1014721	3752909	9840311
Chebyshev	476687	1390683	4833439	370915	977976	1849050

50+3**2**,3

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Table 5-2: Work required to reduce relative residual by factor 1.2 6.

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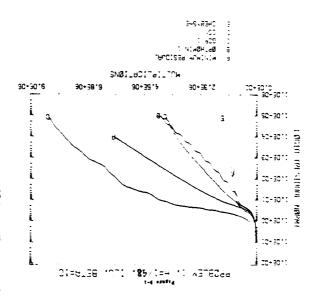
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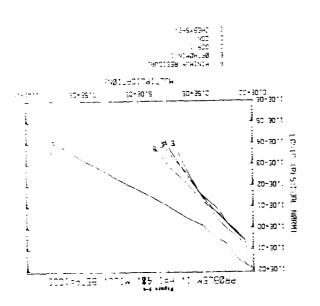
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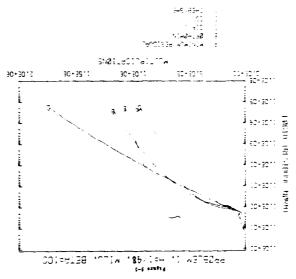
<b>*</b>	32	8	3	32	20	3
9	238643	XOTON S	1914733	27 5457	977681	2478153
Orthonia (1)	290445	1091213	2911573	336021	1196405	3227213
Orthonin(5)	469253	2312901	5600493	442525	1573989	4492893
GCB(1)	291989	991793	2420901	291989	963357	2243425
600(5)	446385	1929545	5641261	401581	1514549	3907113
CGN	666993	2597274	7576986	558328	1793354	4317791
Chebyshev	206677	646156	1597302	300142	1098061	2195291

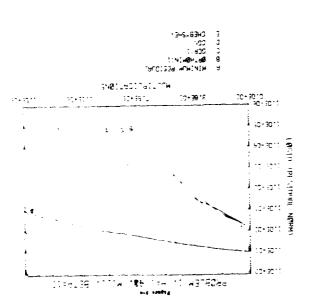
Table 5-3: Work required to reduce relative residual by factor 1.E o Problem 1, Beta = 1000

		;				
٩/١	32	<b>*</b>	99	32	*	•
~	164685	465833	1043993	115453	196804	1043993
Stbomin(1)	184101	530189	1207117	138525	460061	1207117
Orthomin(5)	255429	650349	1613133	175245	5K8773	1013133
GCR(1)	169681	420293	985597	126989	420293	1048725
JCB(5)	212169	\$79165	1366653	149289	550929	1366633
NO.	340998	888944	2054473	319265	939189	2255539
Chebyshev	175522	430003	991368	113212	381969	904806









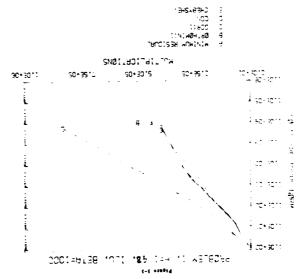


Table 5.4: Work required to reduce relative residual by factor 1.H b. Problem 2, Bota  $\leq 10$ 

1/1	32	<b>*</b>	94	32	<b>7</b>	5
-	1112401	5726493	>15000000	300073	949245	2170833
rthonin(1)	746205	3089861	8719349	229677	635381	1333373
thouta(5)	977085	3174965	8369493	362341	1019805	2166933
G(2)(1)	676989	3376357	10705177	236989	645857	1442989
(2)	752905	2441182	515532!	284473	820965	1666797
3	1471114	7169569	18169347	175658	2647519	6581123
Chabyshev	518227	2106775	5008563	391685	929942	1805769

Table 5-5: Work required to reduce relative residual by factor  $1.E^{\prime}6$  . Problem 2, Beta  $\sim 100$ 

	1	23			N.T.U	
1/1	32	87	*	32	90 4	***
	300073	977681	2119613	287765	949245	227327
Orthonin(1)	336021	11 26 405	3164085	381597	1301597	3164085
Orthonia (5)	683077	2436053	5822013	549437	698 IRRI	493593
(1)	307181	1090357	2763945	334681	1090357	147212
(2)(2)	539649	2006301	4582437	473113	1659509	409649
3	601794	2295804	6762189	536595	1743109	404019
Chebyshev	258602	766241	4316067	464380	1290197	271467

Table 5-6: Work required to reduce relative residual by factor  $1.\,\mathrm{k}^{-6}$  . Problem 2, Beta  $\simeq 1000$ 

		a <b>:</b>			2	
1/1	32	84	3	32	*	*
	373921	1176733	2939133	336997	1318913	4424513
rthonin(1)	396789	1406789	3542853	411981	1722365	6131101
bribonia(5)	576165	2251325	5489733	549437	2682357	7483413
(1)	346989	1118793	2649597	346989	1344357	3678729
GCB(5)	500613	1929545	4021461	473113	2171145	5740113
35	601794	1893844	4498864	688726	2094824	4951529
Chebyshey	403992	1410282	3060918	424762	1482333	3450447

